Exascale, a great opportunity for Clean Energy Transition in Europe

About EERA

The European Energy Research Alliance (EERA) is the association of European public research centres and universities active in low-carbon energy research. EERA pursues the mission of catalysing European energy research for a climate-neutral society by 2050. Bringing together more than 250 organisations from 30 countries, EERA is Europe's largest energy research community. EERA coordinates its research activities through 18 Joint Programmes and is a key player in the European Union's Strategic Energy Technology (SET) Plan.

About EoCoE

At the crossroads of the energy and digital revolutions, EoCoE develops and applies cutting-edge computational methods in its mission to accelerate the transition to the production, storage and management of clean, decarbonized energy. Financed as project EoCoE-II with the support of EU under grant agreement no. 824158.

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toward exascale for energy

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Exascale, a great opportunity for Clean Energy Transition in Europe

Joint EERA-EoCoE position paper on HPC for Energy

Endorsement

This position paper delivers key messages for both the scientific community and policymakers in the EU. It highlights the crucial role that high-performance computing (HPC) plays in delivering on the goals of the EU Green Deal, supporting the green and digital transitions in Europe. HPC is undoubtedly at the core of scientific, industrial, and societal advancements, especially when it comes to designing solutions for complex and multi-disciplinary challenges, such as Clean Energy Transition.

For the scientific community, this paper is a clear call for increasing the use of HPC in addressing a range of R&I challenges in clean energy research. For the policymakers, it provides key recommendations for improved funding and coordination of actions, fostering HPC excellence and competitiveness in the EU.

Adel El Gammal, EERA Secretary General

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Executive summary

Given the positive auspices of the EU policy agenda in the energy sector linking the strategy to accelerate decarbonisation with the adoption of digital technologies, the European Energy Research Alliance (EERA) jointly with the Energy oriented Center of Excellence (EoCoE)[1] presents to the European Commission this position paper on *Exascale, a great opportunity for Clean Energy Transition in Europe*. As Europe is working towards a decarbonized energy ecosystem, with a clear vision and goals set by the European Green Deal, EERA and EoCoE have identified a blind spot: energy domain scientists do not take full advantage of the potential that HPC-fueled simulations can offer to their work! This situation is the result of a lack of HPC related expertise available to scientists. To this end, EERA has recently created a transversal Joint Programme "Digitalisation for Energy" that allows a wide range of scientists in the energy domain to access the considerable expertise amassed through previous cross-domain collaborations between application experts and domain scientists explored in the project EoCoE. Currently, a few pilot collaborations are already established via this Joint Programme (in materials modelling, hydropower and energy systems integration) and more are to follow.

The position paper aims to trigger **suitable coordination actions and funding decisions** from the European Commission and Member States to support the development of tuned data models and simulation codes for energy thematic areas, while making use of the latest technology in High-Performance Computing (HPC) and Data management becoming available at EU level: the Exascale generation. The paper explores the role played by digital tools tuned for the energy sector in support of the transition towards climate neutrality. With a special focus on the computing field, it will detail the current status, the integration of digitalization for energy in the European policy strategy and funding schemes, as well as the challenges faced by this innovative endeavour. It will also delve into EERA's approach and the new Joint Programme, address EoCoE's role within this framework, and provide strategic recommendations. These recommendations are intended for national and European funding entities, and for the energy scientific community as a whole.

The political commitment[2] expressed by the European Union to participate and win in the race for the development of the most performant Computing and Artificial Intelligence technology (as compared to other world regions) has justified supporting the development of research infrastructure in high-performance computing. Scientific communities can now have access to the most powerful computing resources and used these to run simulations focused on energy challenges. Simulation enables to plan for and work towards the clean energy sources of tomorrow in a digital framework, reducing considerably prototyping waste and costs.

While the European Union's financial support has been clear and steady, and remains so under the newly-founded framework of the EuroHPC Joint Undertaking, it has also been insufficiently coordinated in calls for projects financed by DG Energy and calls for projects financed by DG Communications Networks, Content and Technology. In addition, coordination between funding by the EU and by national funding agencies in these areas is a must but is not implemented in a practical way. The lack of a unified strategy and responsive coordination

[1] See for more information the web sites of the EoCoE project and of the EERA association.

[2] See more information on the EU Policy documents «Path to the Digital Decade» and the «Digital Compass» here.

must be rectified since cross-cutting and multidisciplinary activities are crucial to making the most of the computing tools and progressing towards a less carbon-based energy ecosystem.

Having assessed the potential of digitalization as an asset for energy research, and studied the current successes and shortcomings of the application of digitalization to energy domains, EoCoE and EERA have been working hand-in-hand to set up a transversal Joint Programme to promote and streamline how digitalization as a whole, including but not limited to HPC and simulations, is used. Users are, first and foremost, scientists working on energy domains, but also industrial actors in a position to exploit the scientific results having reached their full potential.

This transversal EERA Joint Programme ‘Digitalisation for Energy’, launched in October 2020, was designed as a cross-cutting structure to the other EERA Joint Programmes with the aim of leveraging pre-existing expertise within the established EERA structure and of complementing it with leading edge knowledge on the latest digital concepts and technologies. As the focus on transdisciplinarity and community building are mainstays of the programme, it promotes and fosters transdisciplinary collaborations across all EERA activities.

EERA and EoCoE are confident that this Joint Programme will be an important asset for research and industry energy communities. It will provide the tools and expertise to run energy-focused simulations on large scale systems, thus fully exploiting the immense potential of high performance computing; ultimately, this Joint Programme will play an important role in changing Europe’s energy ecosystem.

As a preview of what this position paper entails, here are the main recommendations that EoCoE and EERA would like to convey to EU and national funding authorities as well as to research and innovation stakeholders:

Current situation

Lack of a unified contact point to discuss HPC and digitalization in the framework of the energy transition, as several European policy DGs cover an aspect of the topic.

Recommendation

Improve coordination at EU level in the context of funding programmes on HPC and digitalisation for energy transition to clean energy sources.

Having a clear contact point to discuss HPC-fuelled simulations at DG Energy, and, in the same spirit, it would be ideal to have a dedicated contact point at DG Connect to discuss energy-specific applications.

Current situation

Without a clear policy framework that links HPC technological innovations with suitable Energy applications, funding is directed to support either scientific or computing advancements with no support for trans-disciplinary collaborations and knowledge transfer to industry.

Recommendation

Structure and consolidate expertise in the energy scientific community at EU level, and even more so where transdisciplinary collaborations are to be encouraged. **Long-term planning for investments in HPC for Energy** is a must.

Keeping in-house experts on long-term contracts, thus limiting loss of knowledge and skills, would allow scientific teams to position themselves more comfortably for stable cooperation and collaborative endeavours, therefore significantly increasing their scientific output.

Current situation

The Energy-oriented Centre of Excellence opened the path for four Energy application domains to collaborate with mathematicians, computer scientists and computational scientists in order to design the best computer workflows for their scientific challenge. The funding is directed to applications that require huge amounts of computational power, whereas many other use cases would also require this collaborative work to be supported.

Recommendation

Align Energy application domains with HPC technologies in order to maintain current trans-disciplinary collaborations as the source of expertise for improved scientific advancements.

EERA's transversal Joint Programme 'Digitalisation for Energy' relies, thus, on an evolution of the funding schemes coming from the energy application domains as an important step towards achieving the programme's goals. Having the energy application domains dedicate funding to activities in line with the programme's objectives would strengthen the whole endeavour, as it would send a clear signal to Energy application domain teams that joining forces with HPC-focused teams is a widely accepted path towards expanding their work and maximizing their impact.

Introduction

The European Commission sets with the European Green Deal an ambitious policy agenda in the energy sector, whereby Member States first milestone is to reduce their greenhouse gas (GHG) emissions by 55% by 2030[3]. In March 2021, the European Commission proposes the “2030 Digital Compass”[4], a strategy that aims to translate EU’s digital ambitions into clear, concrete targets and bring the political impetus to accelerate Europe’s digital transformation. The strategy establishes a monitoring system and outlines key milestones as well as the means to achieve them.

The European Union (EU) has ambitious goals for the supercomputing domain, having created the EuroHPC Joint Undertaking (JU). The EuroHPC JU is a legal entity that coordinates efforts and pools the resources of the European Union and EuroHPC JU’s participating states to deploy world-class supercomputers[5].

The European Energy Research Association (EERA), representing the largest energy research community in Europe, recognized recently the critical and transformative role that the *digitalisation of energy* plays in supporting the transition towards climate neutrality by 2050[6]. To this effect, EERA formally launched a new Joint Programme on Digitalisation for Energy (DfE)[7]. This new Joint Programme (JP) is conceived as a transversal (tJP) structure for maximizing the impact of digitalisation as a cross-cutting activity within EERA, constituting a new concept that could be later addressed by new initiatives, if the opportunity arises. Hence, **digitalisation is perceived as an opportunity and an enabler that will connect energy technologies in a cross-cutting and holistic fashion**. The tJP DfE aims at defining key priorities for this field that will derive in research activities and act as a contact point with major European initiatives on supercomputing, big data, artificial intelligence, open science, etc. It will also tackle the European Digital Strategy, which is strongly pushing these IT services.

Data modelling and Simulation are one of the main priorities of the new Joint Programme. The first thematic areas that joined actions with DfE are energy systems integration, hydropower, materials for energy and nuclear materials monitoring. More thematic areas are to join forces with DfE as the programme matures and gets to be better known by the community.

Given the positive auspices of the EU policy agenda in the energy sector combined with the strategy to accelerate the adoption of digital technologies, EERA jointly with the Energy oriented Center of Excellence (EoCoE)[8] decided to present to the European Commission this position paper on *Exascale, a great opportunity for Clean Energy transition in Europe*. The recommendations in the paper apply to all the thematic energy areas coordinated by the existing eighteen Joint Programmes in EERA.

[3] See Clean Energy factsheet published by the European Commission on December 11, 2019.

[4] See “2030 Digital Compass: the European way for the Digital Decade”, COM(2021)118 of March 9, 2021.

[5] Supercomputers are computing devices able to run calculations at 1015 floating-point operations per second (Petascale supercomputers) and at 1018 floating-point operations per second (in near future Exascale supercomputers).

[6]See EERA’s White Paper on the Clean Energy Transition,(Oct. 2021). The white paper identifies as one of the main drivers of accelerated digitalization of the energy sector the availability of High Performance Computing and modelling application codes.

[7] See press release of the EERA Association on December 15, 2020.

[8] See for more information the web sites of the EoCoE and EERAdata projects.

The position paper aims to trigger suitable coordination actions and funding decisions from the European Commission and Member States to support the development of tuned data models and simulation codes for energy thematic areas making use of the latest technology in High-Performance Computing (HPC) and Data management offered by the EuroHPC JU[9].

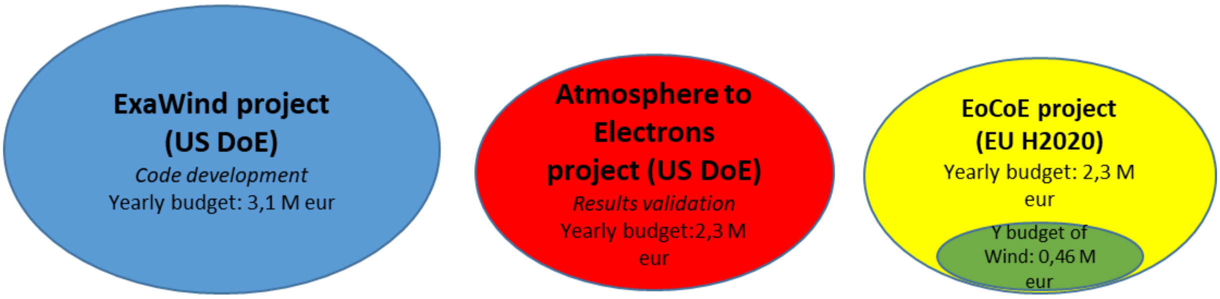
The technical and scientific communities are represented via EERA and its tJP DfE as well as via the two important projects, EoCoE and EERAdata. While the former is largely described along this document, a short description of the latter for the sake of completion follows. EERAdata[10] focuses on supporting policy decisions and renovation action to prioritise investments in energy efficiency counting on a defined work plan. Assess and quantify relevant technical, economic, socio-economic, and environmental variables, indicators and impacts across relevant sectors; develop the appropriate methodology and data analysis framework to plan and compare investment and impact in energy efficiency; and, build a decision-support tool enabling policy makers to plan and prioritise energy efficiency investment.

[9] The High-Performance Computing infrastructure will be funded via the EuroHPC Joint Undertaking (JU). Other ICT-based research infrastructures, like GEANT and EOSC, are also of great importance to the development of simulation codes and applications.

[10] https://www.eeradata.eu/

Part I - State of the art

Tuning of simulation codes and development of new data models for studying specific energy-related physical phenomena lacks, at present, adequate investments. Despite its immense potential, data modeling and simulation is not yet recognized as a vital asset for societal challenges in the provision of clean energy. This state of affairs needs to change if we are to achieve the Green Deal objectives of reaching net zero by 2030 In this paper, we will focus mainly on data modeling and simulation that requires Exascale HPC[11] infrastructure.



Box 1 - Budgetary comparison between projects ExaWind and Atmosphere to Electrons projects[12] funded by US DoE and the budget for the Wind application area in the EoCoE project funded by EC H2020.

EU policies for HPC and energy

Up to now, support for the development of research infrastructure in high-performance computing (HPC) and high-throughput computing (HTC) has been justified by the strategic need to participate and win in the race for the development of the most performant Computing and Artificial Intelligence technology as compared to other world regions (mainly the United States, China and Japan). The differences between HPC and HTC become less and less prominent nowadays and application developers use such data processing technology as required, often via complex workflows that combine both HPC and HTC resources.

With the creation of the EuroHPC JU, the energy research community trusts that, in Europe, HPC/HTC will peer with the most performance computing systems in the world (the Exascale computers). With suitable access to such computing technology, the community can exploit its calculus possibilities to simulate the Clean Energy systems of tomorrow, while improving the

[11] The term «Exascale HPC» infrastructure used in this paper includes supercomputers as a whole : the current petascale and and pre-exascale machines, and the upcoming exascale ones. See the ETP4HPC annual report, page 16, for more information on the European supercomputers.

[12] Here is an example of funds available at both sides of the Atlantic for the development of simulation applied to wind energy production. In Europe, the main effort in tuning HPC codes for renewable energies towards Exascale is the EoCoE project with a budget of 2.3 Million Euros per year, shared among five domains: weather forecasting of extreme weather events, fusion energy, hydropower and geothermal power, new materials for photovoltaics and wind energy. Approximately 0.46 Million Euros per year per domain. Instead, in the US, there are two tightly coupled projects (both directed by Michael Sprague) working specifically on wind energy. The ExaWind Exascale computing project with a budget of 3.5 Million Dollars a year and the Atmosphere to Electrons High-Fidelity modeling project, 2016-2023, with a budget of 2.5 Million Dollars a year. Numbers speak for themselves.

Energy sources of today, and all this in a digital framework that helps reducing prototyping waste and costs.

The challenge ahead of the community is that European Research Framework Programmes offered up to now a very fragmented support to data modeling and simulation in the energy sector.

Investments in research and development were not properly quantified and, thus not properly coordinated by the different EU[13] and national funding bodies. This coordination is a must now that cross-cutting and multidisciplinary activities are an absolute necessity. Attempts to do so have already taken place, but these attempts had no long-term strategy nor a precise follow-up. Under the framework of Horizon Europe, funding for data modeling and simulation will be administrated by the EuroHPC Joint Undertaking. The next call to which the community can participate, in support of European Centers of Excellence in HPC applications, will probably open in the last quarter of 2021. The current Energy oriented Center of Excellence (EoCoE) will end in mid-2022.

The EuroHPC Joint Undertaking funds projects on data modeling and simulation for key application areas (energy is one of these areas) as well as the state-of-the-art infrastructure and tools to promote the use of digital technology (namely of the upcoming Exascale HPC systems). However, such investments target HPC technology advancements in Europe and not its impact on clean energy transition challenges per se. In addition to this, in Cluster "Climate, Energy and Mobility" of Horizon Europe, the focus is on the adoption of digital technologies, not specific to simulation and data modelling topics.

At present, energy-related research exploits Big Data techniques in order to model a wider ecosystem in data-driven simulations encompassing data either previously stored or being measured on-the-fly. The needs of this highly demanding simulations in terms of computational resources (HPC) and data processing/artificial intelligence methodologies requires Exascale supercomputers to exploit the resulting complex workflows. Thus, both HPC and high-throughput computing (HTC) infrastructure is required for simulation codes to compute trustable and accurate results. We refer to the EERAdata project promoted paper "Advancing FAIR metadata standards for low carbon energy research"[14] for a deep study on the topic.

How has the problem been addressed in the past?

Research and development on data modelling and simulation codes received funding in Horizon 2020 of the order of 132 Million Euro[15]. Amongst the 24 awarded Centers of Excellence, the Energy oriented Center of Excellence (EoCoE) received 5.4 Million Euro in

[13] In the Digital technologies sector, DG Connect administrates funding for the Centers of Excellence and Centers of Competence in HPC applications and the implementation of the ICT-based research infrastructure. In the energy sector, funding for research projects is available between various EC bodies, mainly DG RTD and DG Energy with no visible coordination with projects funded by DG Connect in the energy sector.

[14] A. Wierling *et al*. "Advancing FAIR metadata standards for low carbon energy research". Submitted to Energy Strategy Reviews.

[15] Call E-INFRA-5-2015 with 40 Million Euro financed nine Centers of Excellence: see the press release of the launch of the Centers of Excellence on 26 September 2016. Call INFRAEDI-02-2018 with a budget of 72 Million Euro financed ten Centers of Excellence: see the press release of the launch of the Centers of Excellence on 14 June 2019. The Energy oriented Center of Excellence, EoCoE, received funding from the two formerly quoted calls for proposals. Call INFRAEDI-05-2020 with a budget of 20 Million Euro financed five other centres of excellence (see more details here).

2016 for the first three-year project and subsequently 8.3 Million Euro for the following three years up to the end of 2021[16]. Funding amounts to roughly 2.3 Million Euro per year. In addition to this, access to the required HPC resources and services for testing and benchmarking of codes was available via the PRACE research infrastructure. The funding of the projects EoCoE and EoCoE-II enabled for tuning the flagship codes of each of the five energy application areas (materials, wind, water, fusion and meteorology) to fit exascale computing power and, not to be underestimated, created the basis for a sound and profitable collaboration between computer and computational experts, mathematicians and scientists of each the application areas.

The FocusCOE project, the coordination and support action[17] of all Centers of Excellence, has received two Million Euro funding for three years. EoCoE and all the other funded Centers of Excellence benefit from this coordination support action. FocusCOE acts a link between CoEs, a discussion space to collect and relay best practices, recommendations and updates on every CoE's work; it coordinates CoEs participation to events and fairs, and encourages collaborations between CoEs based on their scientific topics and objectives. Thanks to the collaboration with FocusCoE, EoCoE submitted a joint participation to the European Union Sustainable Energy Week (EUSEW) in 2021. The proposal was accepted and marked the first attendance of the CoEs at EUSEW. FocusCoE provided also an online space where the codes of each of the CoEs are presented and classified by topics and application domains[18]. This provides a greater visibility to the resources and expertise in Europe on high-performance computing.

HPC, simulations, massive data treatment as a driver for innovation towards energy transition

The aforementioned creation of the EuroHPC JU and the "2030 Digital Compass" strategy underlines that the EU sees digitalization as a fundamental part of Europe, both on a societal, technical, and economical level. The European Green Deal, an unquestionably ambitious approach to fight against climate change and environmental degradation, attests to the EU's leadership in face of the 21st century's greatest challenge.

Thus, there are several examples in which the advances that the exploitation of digital methodologies can bring will produce the resolution of more ambitious problems in the energy sector. Some of those will be described in more detail below, but in what follows, an itemized non-complete list of energy topics to be approached with proper digital techniques reads:

- Improvement in the exploitation of energy sources
    - Weather forecast or turbines in off-and on-shore wind energy
    - Design of new devices such as wind turbines, solar thermal plants, collectors, solid state batteries etc.
    - Computational Fluid Dynamics (CFD) analysis of heat transfer between solar radiation, materials, and fluids

[16] Project EoCoE-II, Grant Agreement number 824158.

[17] Call INFRAEDI-02-2018 with 1.997 Million Euro, for the 01/12/2018 - 30/11/2021 period.

[18] See https://www.hpccoe.eu/technological-offerings-of-the-eu-hpc-coes-2/codes-and-software-packages/

- Design of advanced materials of energy interest
  - Materials for innovative batteries via accurate molecular dynamics and/or ab initio simulations to design and characterize at the atomic-scale new cathodes and electrolytes.
  - Materials for photovoltaic devices via multiscale simulations where atomic-scale ab-initio simulations are combined with mesoscale approaches to design efficient energy harvesting devices.
- Energy distribution
  - Integrated energy system analysis, optimization of the energy mix and smart grids fed with renewable energies, and further distribution in the electricity grid
  - Economic energy models
  - Smart meters and sensor deployment and further application to energy efficiency in buildings, smart cities, etc. Exploitation on additional infrastructures such as fog/edge computing.
  - New actors (prosumers) in a distributed electricity market, including energy systems integration.

Behind all the previous items, there is a solid track of research that forms the foundations of this effort in reinforcing research on digital topics. Some examples are:

- Design of Digitalized Intelligent Energy Systems, for example, their application to cities in which zero emissions buildings or intelligent power systems are pursued
- Deeper understanding of the physics behind the energy sources, for example, multiscale simulation or of the atmospheric flow for wind farm operation through CFD–RANS or LES simulation coupled to mesoscale models taking advantage of the capabilities offered by exascale computing.
- New designs of Fluids Structure Interactions (FSI), for example, for full rotor simulations coupled to Computational Fluid Dynamics (CFD) simulations. Structural dynamics (fatigue) in different devices, which affects almost every EERA Joint Programme.
- Optimization of codes by the means on new mathematical kernels, not simply computational porting
- Integration of different computing platforms seamlessly combining HPC, HTC, and High-Performance Data Analytics methodologies

Moreover, the advanced modelling of energy systems is allowed thanks to the tight synergy with other disciplines from mathematics to computer science, from data science to numerical analysis. Among the other high-end modelling requires:

- Data Science, as handling large volume of data is key to energy-focused HPC and HTC simulations and data-driven workflow
- Designs of customised machine and deep learning techniques for improved artificial intelligence approaches
- Efficient implementation of digital platforms, their interconnections and interoperability

Part II - Successes & challenges

Demonstrating the approach's viability: EoCoE's achievements

This section presents case studies 1 to 4 that stem from EoCoE collaborations. The goal is to present EoCoE success stories that best exemplifies how a Center of Excellence fosters collaborations between experts from complementary fields.

Case study 1: HPC for Wind Energy with Alya

The key to achieving the wide-scale deployment of wind energy is enabling a new understanding of and the ability to predict the fundamental flow physics and coupled structural dynamics that govern whole wind plant performance, including wake formation, complex-terrain impacts, and turbine-turbine interactions through wakes. Current methods for modeling wind plant performance fall short due to insufficient model fidelity and the inadequate treatment of key phenomena combined with the lack of computational power needed to address the wide range of relevant length scales associated with wind plants[19].

Fragments to trigger further discussions:

- Skills and R&D: HPC for Wind Energy competes with projects "Atmosphere to Electrons" and "Exawind projects" (in the USA) with a much inferior budget (see Box 1).
- To Out Compute is To Out Compute: Can Europe be a leader in Wind Energy if European Wind Experts plan to adopt US developed applications. Note that there are robust EU applications on this domain!
- Work force: often on temporary contracts! Hard to attract new talents.

Success stories*:*

- Wind plant losses are estimated at 20% on flat terrain and higher for complex terrain. Reducing losses of power by 1% means already huge savings. High fidelity computational fluid dynamics simulation is one of the best tools for this.
- The scientists in this case study[20] are world leaders in WMLES for Complex geometry. There is a strong interest in industrial usage of the code and subjacent methods. Collaboration with Iberdrola on wind energy for already 10 years.

[19] See also for more information: https://www.exascaleproject.org/research-project/exawind/

[20] H. Owen; G. Chrysokentis; M. Avila; D. Mira; G. Houzeaux; R. Borrell; J.C. Cajas; O. Lehmkuhl, « Wall-modelled large-eddy simulation in a finite element framework, Intl. Journal Numerical Methods in Fluids, Vol. 92, Issue 1 (Jan 2020), pages 20-37, https://doi.org/10.1002/fld.4770.

Contact: Dr. H. Owen and Dr. O. Lehmkuhl (Barcelona Supercomputing Centre).

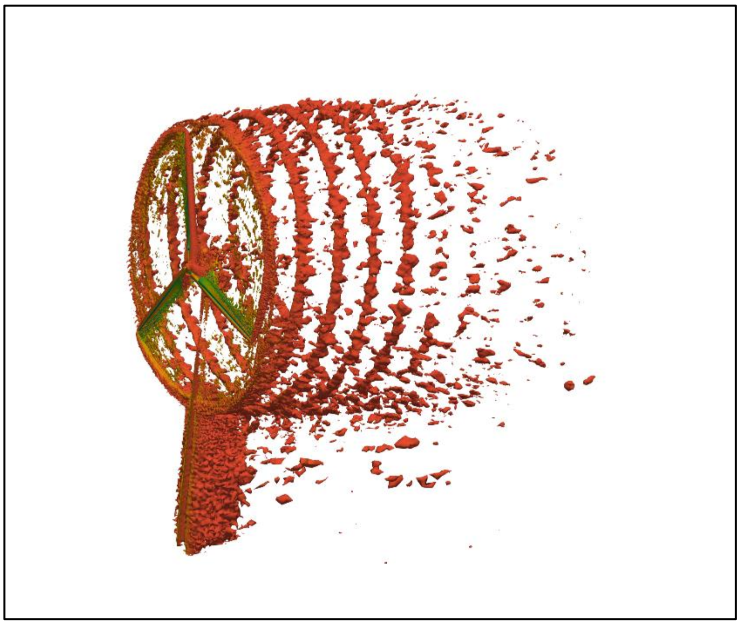


Figure: Full rotor simulation with code Alya including mast, nacelle, and rotating blades.

Case study 2: HPC for Solid-state Batteries and Photovoltaics

The key to achieving the wide-scale deployment of electrical storage is enabling a new understanding of and the ability to predict the physics of solid-state batteries that governs both energy storage and charging rates. Solid-state batteries are safer, easier to process, have higher achievable power density and cyclability than conventional liquid-state batteries. This case study is a collaboration between materials scientists, mathematicians and data analysts.

Success story:

Predicting the equilibrium distribution of charged ions within crystalline solids at, or near, structural discontinuities such as grain boundaries or heterointerfaces is a long-standing problem in solid-state physics. Polycrystalline solids exhibit material properties that differ significantly from those of equivalent single-crystal samples, in part due to a spontaneous redistribution of mobile point defects into space-charge regions adjacent to grain boundaries. The spatial profiles of space-charge regions are particularly significant in solid electrolytes such as those used in solid-oxide fuel cells and all–solid- state lithium-ion batteries. We find unexpected oscillatory behaviour of the defect density near a grain boundary shown in the figure below[21]. A local decrease in the concentration of the charge-carrying mobile ionic species within a space-charge region is expected to contribute to interfacial resistance and decreased device performance.

[21] J M Dean , S W Coles , W R Saunders, A R McCluskey, M J Wolf , A B Walker, B J Morgan Phys Rev Lett **127** 135502 (2021).

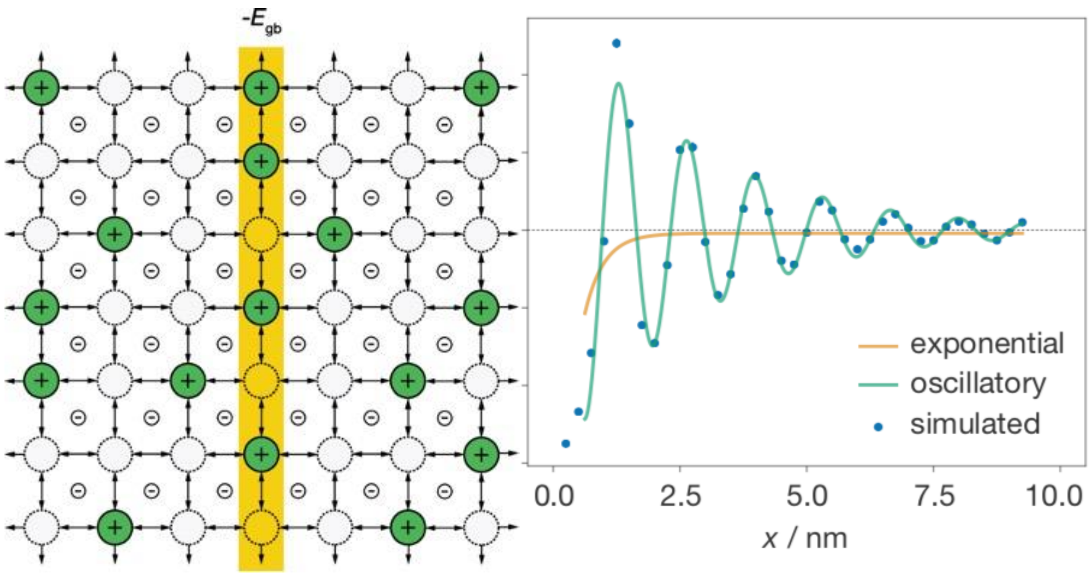


Figure:

- *Left panel: Kinetic Monte Carlo model, central plane (yellow) is a grain boundary (GB)*
- *Right panel: Mobile defect concentration profile near GB. Simulations (filled circles) are compared with maximum likelihood exponential (red line), oscillatory (green line) models.*

Current methods for modelling battery performance fall short due to insufficient model fidelity and the inadequate treatment of key phenomena combined with the lack of computational power needed to address the wide range of relevant length scales associated with charge transport in batteries. Instead of solving an effective one-dimensional problem, we consider an explicit three-dimensional Hamiltonian for point charges in a system with a single grain boundary. We then sample the configuration space of this model by kinetic Monte Carlo simulations, and construct space-charge profiles as time averages over simulation trajectories. Because this approach treats defect-defect interactions explicitly in three-dimensional space, defect-defect correlations emerge directly from the simulation trajectories. To characterize and quantify the simulated space-charge profiles, we performed maximum likelihood sampling, parameter posterior sampling, and Bayesian model selection for competing functional forms

Our approach solves a major materials problem and addresses electrostatic interactions in heterogeneous systems in a completely new way by employing a fast multipole solver[22]. It is implemented by “Separation of Concerns” used in the development of parallel and optimised MD codes[23]. Here, the science specialist writes code at a high abstraction level in a domain specific language which is then translated into efficient computer code by a scientific programmer. Python code is generated for simulations on different parallel architectures, including massively parallel distributed memory systems and GPUs.

Contact: Prof Alison Walker (UBAH, University of Bath).

[22] W. R. Saunders, J. Grant, E. H. Müller, I. Thompson, J. Comput. Phys. **410**, 109379 (2020).
[23] W. R. Saunders, J. Grant, E. H. Müller, Comput. Phys. Commun. **224**, 119 (2018).

Case study 3: HPC for Pan-European Hydrological Modelling with ParFlow

The accurate prediction of stream discharge, including its variability and uncertainty, is key in reservoir management for hydropower production. The discharge information is required at extremely local space scales with high temporal resolution over large regions with strong topographic relief. In addition, long-term projections are required in order to assess the increase in discharge variability due to climate change. This is only possible with detailed hydrologic models providing relevant, local information over regional to continental scales.

This case study uses ParFlow hydrologic and hydropower production models to simulate hydrologic states and fluxes relevant to the energy sector. ParFlow is a massively parallel, physics-based integrated hydrlogic model and simulates fully coupled dynamic 2D/3D hydrological, groundwater and land-surface processes for large scale problems[24]. ParFlow is a highly scalable code enabling it to be used for high resolution simulations ranging from single river catchments to continents. ParFlow is successfully run on a large range of platforms ranging from single CPU notebooks and workstations to distributed/shared memory clusters (e.g. JSC/JURECA) to massively parallel systems such as JUWELS Booster Module supercomputer at the Jülich Research Center.

Furthermore, detailed simulation of hydropower systems functioning was performed and validated in the Italian Alpine region by means of HYPERstreamHS model.

Success story:

- The graphics processing units (GPUs) were implemented with the ParFlow code to accelerate model performance in simulating the three-dimensional variably saturated groundwater flow and overland flow[25].
- The implementation for accelerator architectures in ParFlow hydrologic model shows a good scaling across multiple nodes with 15-16 times increase in the performance from using GPU accelerators.
- HYPERstreamHS hydrological model[26] was developed and tested in order to simulate the presence of human infrastructures in large river basins.

The figures below showcase the map of Pan-European domain showing, from left to right, average precipitation, soil moisture, water table depth distribution and evapotranspiration (1997 - 2006) over Europe and in Alpine (red box) region estimated by ParFlow-GPU model. Validation[27] of the Hydropower Production module (HPP) was performed at monthly time scale in several sub-basins located in the Italian Alpine region (see pictures below).

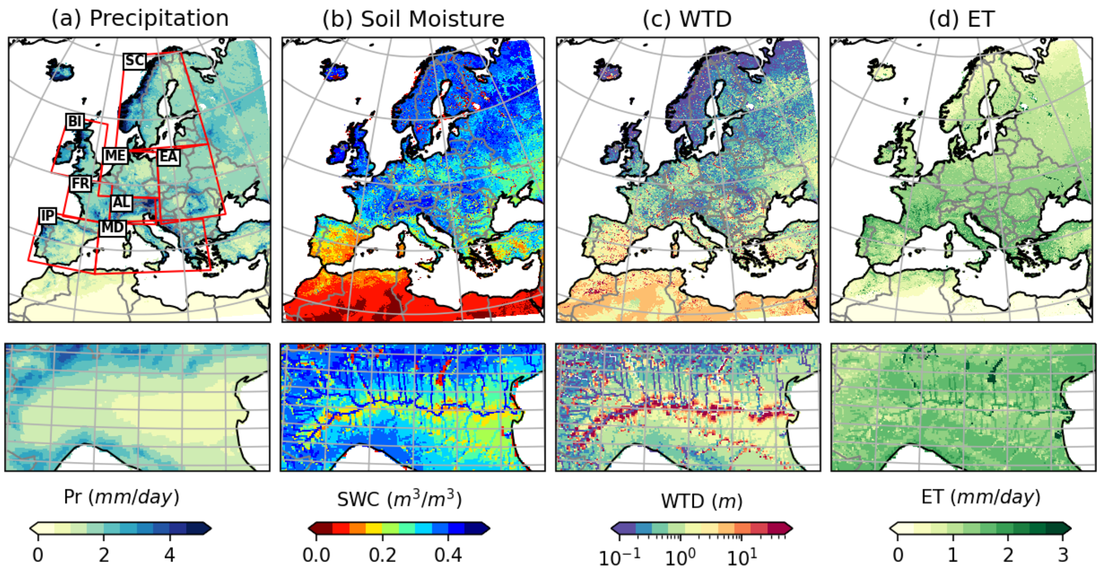
[24] S. J. Kollet and R. M. Maxwell: Integrated surface-groundwater flow modeling: A free-surface overland flow boundary condition in a parallel groundwater flow model, Adv. Water Resour., **29**, 945–958, https://doi.org/10.1016/j.advwatres.2005.08.006, 2006.

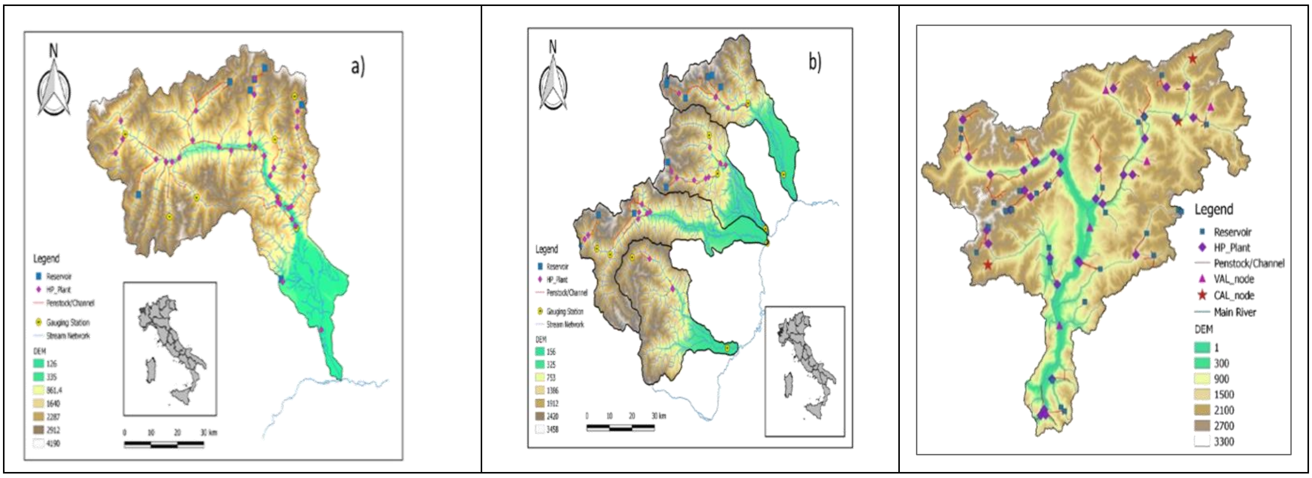
[25] See J. Hokkanen, S. Kollet, J. Kraus, A. Herten, M. Hrywniak, and D. Pleiter, Leveraging HPC accelerator architectures with modern techniques - hydrologic modeling on GPUs with ParFlow. Comput. Geosci., doi:10.1007/s10596-021-10051-4.

[26] See D Avesani, A Galletti, S Piccolroaz, A Bellin, B. Majone, A dual-layer MPI continuous large-scale hydrological model including Human Systems, Environmental Modelling and Software, 139, 105003 (2021).

[27] A Galletti, D. Avesani, A. Bellin, B. Majone, Detailed simulation of storage hydropower systems in large Alpine watersheds, Journal of Hydrology, 127125 (2021).

Contact: Dr. S. Kollet (FZJ), Dr. B. Naz (FZJ) and Dr. B. Majone (Univ. Trento).





Case study 4: Weather forecasting for rare weather events with WRF and ESIAS

Accurate forecasts of photovoltaics (PV) and wind power production are increasingly important to guarantee a stable and economic grid operation with weather-dependent power sources. Weather forecasting for **extreme events and errors in weather forecasts** constitute the biggest problem in the exploitation of energy from PV and wind sources, often offsetting something like a month of profits on energy markets. These events are often far outside of the distribution of any of contemporary o(50) ensemble members in probabilistic forecasting. The main difficulty is in correctly forecasting the correct location of such weather events.

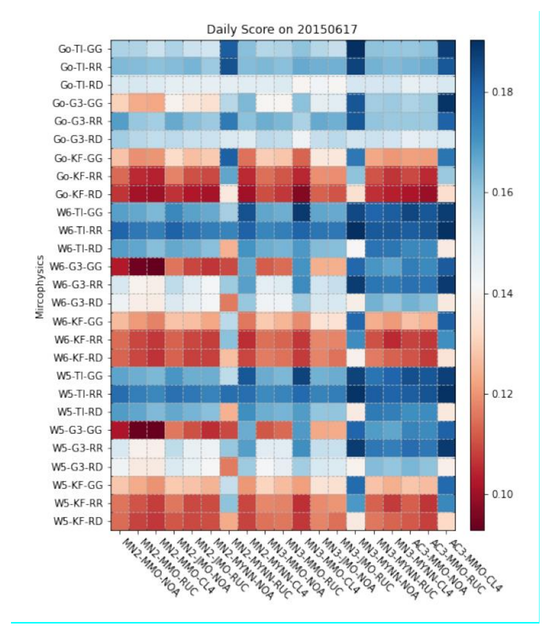
This case study features a collaboration on HPC Ensembles for Renewables Forecasting between meteorologists and HPC technical experts at Forschungszentrum Juelich using HPC for next generation ensemble forecast sizes. The application codes used are ESIAS (Stochastic Integration of Atmospheric Simulations) and the WRF (Weather Research and Forecast Model). Energy application expert Fraunhofer IEE trains and experiments on wind and solar forecasts of unprecedented size a decision support system for planning energy production from renewables.

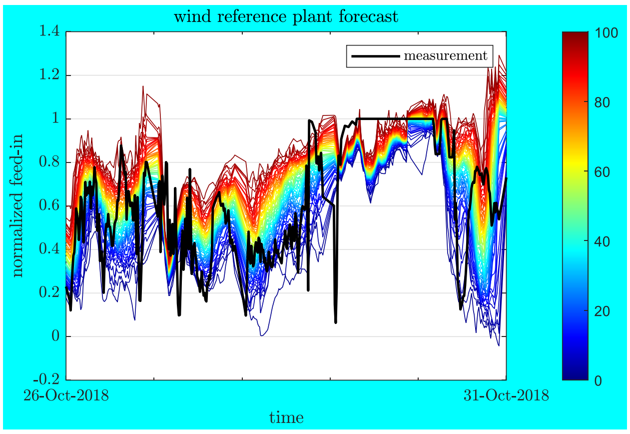
Success story:

- The real success here was the collaboration between Forschungszentrum Juelich and Fraunhofer itself. No one has the resources to run a live forecast at this scale. That's not the goal of the project to create an operational system that will directly affect grid operation. This research focus is to gain important experience on whether we need probabilistic training in the future.
- The collaboration aims to improve the efficiency of algorithms and data input/output to be able to practically handle weather forecasts of this scale.
- A vast number of physical schemes have been tested with the application code ESIAS. The accuracy of the obtained results are being assessed on the ability to affect daily forecasts on wind power generation.

Many model combinations were tested and scored according to daily weather observations for a rare event that occurred between 26.10.2018 and 31.10.2018[28] (left image below). A total of 512 members / years were simulated based on four promising physical model schemes. The forecast for a wind reference plant was well captured by the ensemble distribution (right image below).

Contact: Dr. G Good (Fraunhofer IEE).





[28] See J. Finkenrath; G, Koutsou; S. Metzger; H. Elbern; J. Berndt. (2019). "Approaching Exascale with the Weather Research and Forecasting Solar Model". Zenodo. https://doi.org/10.5281/zenodo.2677532

The EoCoE / EERA Joint Program "Digitalization for Energy"

- *Goal: to maximize the impact of digitalisation as a cross-cutting activity within EERA*
- *Defines key priorities that can be addressed through HPC-fueled simulations*
- *Contact point with major European initiatives on supercomputing, big data, artificial intelligence, open science.*
- *Demonstrates the usefulness and relevance of HPC energy-related simulations as a tool for EU energy strategy*

EERA and EoCoE assessed the potential of digitalization as a massive asset for energy research, and ultimately a steppingstone towards a cleaner, decarbonized ecosystem, and launched an extensive consultation within the EERA community to further determine which domains would be best suited to take full advantage of a transversal joint research programme on digital topics. This consultation process concluded in the fall of 2020, and EERA formally launched the transversal Joint Programme "Digitalisation for Energy" on December 15, 2020. This Joint Programme recognizes the critical and transformative role that the digitalization of energy plays in supporting the transition towards climate neutrality by 2050. As the first transversal programme created by EERA, it was designed as a cross-cutting structure to the other EERA Joint Programmes with the aim of leveraging pre-existing expertise within the established EERA structure and of complementing it with leading edge knowledge on the latest digital concepts and technologies.

The "Digitalisation for Energy" Joint Programme has its own management board; it will integrate, on a modular basis, specific subprogrammes tailoring digital methodologies in a transparent and agnostic way (HPC, data science, artificial intelligence, etc.) and all the existing sub-programmes that, even though belonging to existing Joint Programmes, have already developed a particular expertise in digitalisation topics. The Programme's board will define key priorities, i.e., the challenges that will be addressed through digital capabilities such as, for example, HPC-fueled simulations.

The Joint Programme also aims to become a contact point between the EERA community and the major European initiatives on the topics relevant to its core domains. This includes, but is not limited to, supercomputing, big data, artificial intelligence, cybersecurity, and blockchain. The Joint Programme will also be EERA's entry point for matters pertaining to open science and will therefore participate to the implementation of EU's Open Science policy and tools, among them the European Open Science Cloud (EOSC).

Issues identified so far

As the Joint Programme intensifies its activities, it will have to face several challenges if it is to achieve all of its goals:

Issue 1: ***Fostering transdisciplinary collaborations*** is one of the main objectives of the Joint Programme. To achieve it, EERA and EoCoE are fully aware that they will have to promote collaborations between domains that currently are not speaking enough amongst each other. Direct collaborations between HPC experts and energy domains experts are sparse, as experts tend to join forces for a specific purpose and rarely stay connected beyond a single project. EoCoE's experience in implementing transdisciplinary collaborations will be key to overcome this challenge. Since its inception, EoCoE has been setting up collaborations between energy domain scientists and HPC experts. Scientists need to solve specific problems through HPC simulations and HPC experts help them to improve the simulation tools they use. EoCoE's results are the living proof that these collaborations allow significant progress beyond the state of the art, both for the technical community and the energy domain one (see case studies 1 to 4 above).

Issue 2: ***Joint Programme's role as a demonstrator*** will be crucial, since it will allow for successful collaborations being carried out within its framework to snowball to a large number of scientific communities. The Joint Programme will emphasise the usefulness and relevance of HPC energy-related simulations as a fundamental tool to achieve the paradigm change Europe needs to move towards a decarbonized energy ecosystem. Given the Programme's privileged position, at the intersection of EERA's other JPs and as a contact point with the European Commission, this demonstration of the part simulations can play for the energy domain will have a large-scale impact, both on the extended EERA community and on the EU energy strategy.

Issue 3: ***Scattered funding schemes for HPC technology and its application domains***. Funding schemes that support HPC technology advancements in Europe through EuroHPC are disconnected from HPC's impact on clean energy transition challenges, with the notable exception to this situation being programmes that frame the use of HPC within the European Green Deal. The Joint Programme will have to reconcile both aspects and demonstrate to funding entities, both national and European, that investing on *energy applications* of HPC technology can have a massive impact on the transition towards a clean energy ecosystem.

Issue 4: ***Duration of funding schemes*** is another issue the Joint Programme will have to consider. Fostering collaborations and ensuring they develop on a long term can be a daunting task when funding schemes operate on a two- or three-years basis, as the lack of clarity on a research team's budget and manpower can hinder its perspectives and prevent it to fully engage in the sort of scientific endeavors the Joint Programme aims to promote. Addressing this issue will be part of the Joint Programme's role as a national and European contact point.

Issue 5: ***Outreach to industry applications***. This Joint Programme's role will be to bridge the gap between scientific use-cases and their potential use by industrial actors, and play a significant part in the transfer of expertise between academia and commercial actors. At present, research on data modeling and simulation has not yet sufficiently attracted sustained interest from companies in the energy sector, an issue that can be attributed to technology readiness levels being too low to allow industries to assess their potential returns on investment. There are, of course, exceptions to this rule, as some research teams have been collaborating with industrial companies on market-ready endeavors[29]; but still, these occurrences are far from the norm.

[29] For instance, the Barcelona Supercomputing Center (BSC) has been working with the Iberdrola company, using RANS simulations with the Alya code for their daily simulations. The Juelich research center (FZJ) is also in contact with the transmission system operator Tennet TSO GmbH. JSC contributes knowledge in the field of HPC in order to adapt different applications for parallel processing and to design a parallel computer with intelligent resource management.

Part III - Propositions to bridge the gap between the renewable energy and HPC communities

Based on the elements mentioned above, the Joint Programme's board intends to put forth several proposition to bridge the gap between the renewable energy and HPC communities.

This is very much a time of opportunity, as the European Green Deal sets a clear policy for research in clean energy sources with the support of digital technologies, namely data modeling and simulation[30]. Digital technologies are a real asset within the clean energy transition perspective, and we already have strong scientific results that demonstrate how transdisciplinary collaboration on digitalisation for energy can jumpstart energy-related scientific output. Finally, yet importantly, the two opportunity factors quoted above constitute a significant opportunity as the European economy evolves past the Covid-19 pandemic. A strong pull for stronger collaboration between experts in digital technologies and in energy-related use cases is now necessary for the benefit of European society as a whole, as it reinvents itself in the light of the past two pandemic years.

Fostering cross-domains collaborations

The Joint Programme operates under the certainty that using HPC-fueled simulations as a basis for future scientific achievements requires strong, long-term collaboration between application experts and domain scientists. Fostering said collaboration will be key to the programme's success, and it will not go without its challenges.

To overcome said challenges, current collaborations in project EoCoE will be used as a template to explore what can be achieved within the scope of the Joint Programme.

Cross-domains collaborations should strive to be more than mere single case cooperation, which implies that implementing a long-term strategy will be an important part of the Joint Programme's role. The programme will provide a framework for these endeavors, and integrate them in a global vision that will span across years, as this is the only way to achieve the ambitious goals we intend to.

It bears mention that the Joint Programme will also focus on data, a topic that was not specifically part of previous projects. This situation provides an interesting starting point, as it will allow fostering collaborations at the programme's level, between its original participants.

The role of EoCoE

Since EoCoE played a crucial part in the conception and creation of the Joint Programme, it will naturally shoulder a significant responsibility regarding the programme's deployment.

EoCoE is, and has been for the past six years, a place of collaboration between technical and scientific communities, which will ultimately allow said communities to maximize the usage and the scientific outputs of the future exascale systems.

[30] See EC Communication"The European Green Deal", COM(2019) 640 of 11 December 2019. Digital technologies are a critical enabler for attaining the United Nations sustainable environment goals adopted by the European Green Deal in the energy sector, amongst other sectors.

EoCoE is a large consortium, gathering eighteen members and spanning across seven European countries. Its size is of note, as it demonstrates how important it is to reach a critical mass of researchers to start real long-term interdisciplinary work.

We already mentioned the importance of bridging gaps - between scientific communities, and between academia and industry. Such a feat can only be achieved through frequent, well-publicized, high-level training activities, aimed towards all actors of the field. This can prove a complex task, given how diversified the field is, and the Joint Programme's training activities will have to be calibrated to reach energy domain scientists, HPC applications experts, and potentially industrial actors altogether.

EoCoE's training activities have been a constant part of the project, with sessions directed to the various types of audiences described above. EoCoE will keep providing these training sessions, will advertise them through EERA's networks, and will therefore participate fully to the community-building effort that will take place within the Joint Programme's framework.

Given that previous EoCoE training activities promoting the use of HPC systems have attracted interest outside of the consortium and outside of the academic sector[31], the project's participants will build upon these successes to ensure the Joint Programme's outreach to industries is as efficient as possible.

It should be noted that the EoCoE community is constituted of energy application scientists and HPC experts, which is a combination of expertise that did not exist within the previous EERA programmes. The integration of EoCoE will therefore bring new knowledge to EERA, which opens an opportunity for the EERA community to receive best practices they may not be aware of, and gain access to new tools, new expertise The goal of this integration is that the EERA community seizes this opportunity, sets new scientific objectives, starts new collaborations and maximizes its scientific output.

The large community gathered within EoCoE, and the successes it has achieved over the last five years, is a testimony to what can be done through cross-domains collaboration. It also demonstrates the importance of catering to the diverse needs of the different domains – computer application specialists do not have the same needs as domain experts, and both must be satisfied for the collaboration to bear fruits.

EoCoE's achievements and sustained excellence is also a major argument in favor of keeping the interdisciplinary collaborations alive, and this means not splitting the community built through this consortium. The joint programme is very much a part of EoCoE's long-term strategy and sustainability plan, and it will play a crucial role in guaranteeing the community built through EoCoE keeps working hand in hand.

Considering EoCoE as a large scale proof of concept for what the joint programme can bring to various energy-related scientific groups has been a starting point for this endeavour. It will bring mutual benefits for EoCoe's community, the EERA energy communities, and the European energy ecosystem as a whole.

[31] An example of this is the « EoCoE innovations toward exploitations » workshop (February 2021) and « Pitching EocoE results » workshop (June 2021). Both workshop were organized jointly with META Group and received positive feedbacks from companies (among the others (ENI, Solvay, E.ON and capital ventures).

In this sense, it is a very good example how the EERAdata project is building a common specification of data in the energy domain. Working on standardisation and adoption of FAIR principles designed for the energy sector, the pillars for a common energy data space properly exploited are being defined, which will result in a clear added value for supporting policy decisions to prioritise investments in energy efficiency.

Strategic recommendations

EERA and EoCoE are confident that the Joint Programme Digitalisation for Energy will yield significant results; but they are also aware that some evolutions in the current European ecosystem would further improve the work being done within the confines of the programme.

We mentioned the lack of a unified contact point to discuss HPC and digitalization in the framework of the energy transition, as several European policy DGs cover an aspect of the topic. Having a clearer contact point to discuss HPC-fueled simulations at DG Energy, for instance, would be a boon and in the same spirit, it would be ideal to have a specialized contact point at DG Connect to discuss energy-specific topics.. These changes would streamline the elaboration of future policies and guarantee that HPC technologies are a part of them. We acknowledge that EERA has already worked in this direction and is very much an entry point for scientific communities that wish to convey recommendations of this sort to the European Commission.

Current situation

Lack of a unified contact point to discuss HPC and digitalization in the framework of the energy transition, as several European policy DGs cover an aspect of the topic.

Recommendation

Improve coordination at EU level in the context of funding programmes on HPC and digitalisation for energy transition to clean energy sources.

Having a clear contact point to discuss HPC-fueled simulations at DG Energy, for instance, would be a boon and, in the same spirit, it would be ideal to have a dedicated contact point at DG Connect to discuss energy-specific applications.

We also described how the lack of long-term funding could be a hindrance when it comes to building scientific teams, and an even bigger one when it comes to fostering transdisciplinary collaborations. While EERA and EoCoE acknowledge that funding schemes are a complex topic, they would like to underline that longer funding durations could provide better stability and long-term vision to the programme’s participants. Beyond the elements we previously mentioned, i.e. keeping in-house expertise on longer contracts and limiting loss of knowledge and skills due to a funding coming to its end, longer funding schemes would allow scientific teams to position themselves more comfortably for stable cooperation and collaborative endeavours, therefore significantly increasing their scientific output.

Current situation

Without a clear policy framework that links HPC technological innovations with suitable Energy applications, funding is directed to support either scientific or computing advancements with no support for trans-disciplinary collaborations and knowledge transfer to industry.

Recommendation

Structure and consolidate expertise in the energy scientific community at EU level, and even more so where transdisciplinary collaborations are to be encouraged. **Long-term planning for investments in HPC for Energy** is a must.

Keeping in-house experts on long-term contracts, thus limiting loss of knowledge and skills, would allow scientific teams to position themselves more comfortably for stable cooperation and collaborative endeavours, therefore significantly increasing their scientific output.

Given how the Joint Programme relies on transdisciplinary collaborations as a source of improved scientific production, an evolution of the funding schemes coming from the energy application domains would also be an important step towards achieving the programme's goals. Having the energy application domains dedicate funding to activities in line with the programme's objectives would strengthen the whole endeavour, as it would send a clear signal to application domain teams that joining forces with HPC-focused teams is a widely accepted path towards expanding their work and maximizing their impact.

As mentioned above in the EoCoE-focused section, keeping scientific communities together is very much a crucial need to keep interdisciplinary collaborations going. Splitting communities can be an unintended consequence of specific funding schemes, so we advocate in favour of maintaining or promoting cross-domain work as a priority for future funding schemes, both at the national and European levels.

Current situation

The Energy-oriented Centre of Excellence opened the path for four Energy application domains to collaborate with mathematicians, computer scientists and computational scientists in order to design the best computer workflows for their scientific challenge. The funding is directed to applications that require huge amounts of computational power, whereas many other use cases would also require this collaborative work to be supported.

Recommendation

Align Energy application domains with HPC technologies in order to maintain current trans-disciplinary collaborations as the source of expertise for improved scientific advancements.

EERA's transversal Joint Programme 'Digitalisation for Energy' relies, thus, on an evolution of the funding schemes coming from the energy application domains as an important step towards achieving the programme’s goals. Having the energy application domains dedicate funding to activities in line with the programme’s objectives would strengthen the whole endeavor, as it would send a clear signal to Energy application domain teams that joining forces with HPC-focused teams is a widely accepted path towards expanding their work and maximizing their impact.